J. Chem. & Cheml. Sci. Vol.4 (1), 35-41 (2014)

GC/MS Analysis of Essential Oil Isolated from the Roots of Cymbopogon Winterianus Jowitt

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(Received on: January 10, 2014)

ABSTRACT

Twelve sesquiterpenoids and six known hydrocarbons were identified in essential oil from the roots of Cymbopogon winterianus Jowitt by gas chromatography-mass spectrometry (GC/MS) method, of which the major constituents were α-elemol (32.26%), guaiol (18.81%), methylcyclohexane (9.24%), γ-eudesmol (8.53%), τ-muurolol (6.83%), β-elemene (6.37%), δ-cadinene (4.23%) and (+)-citronellol (2.56%). The essential oil yield and the percentage of identified compounds were 0.16% and 100% respectively. The sesquiterpenoid constituents amounted to 86.58% of the oil. The oil consist several flavor and fragrance compounds and GC/MS findings suggest that the oil may be used in soap, cosmetics, perfumery and food flavoring industries.

Keywords: Cymbopogon winterianus Jowitt, Roots, Essential oil, GC/MS, Sesquiterpenoids.

INTRODUCTION

Essential oils are well known for their flavor and fragrance properties. They have great importance due to their versatile applications in soap, food, cosmetics, perfumery and pharmaceutical industries[1]. Some fragrance oils are widely used in aromatherapy to reduce anxiety, stress, and depression of patients[2], whereas some oils have amazing skin regenerating potential and used in massage after radiotherapy of a cancer patient to reduce its side effects[3]. Essential oils are composed by highly

bioactive molecules and simply isolated from plant parts by steam distillation or hydro-distillation method. Recent investigations revealed the antibacterial, antifungal, antiviral, anti-inflammatory, anti-tuberculosis, anti-carcinogenic, anticonvulsant, anti-nociceptive, anti-hypertensive, analgesic, anti-oxidant, larvicidal and insecticidal properties of essential oils[4-7].

Cymbopogon winterianus Jowitt (Java citronella) is an aromatic plant growing in India, Sri Lanka, Central America, Taiwan, Brazil, Congo, East Africa, Guatemala and West Indies[8]. It is a stemless perennial herb belonging to the Poaceae family of Cymbopogon species. The leaves oil of Cymbopogon winterianus Jowitt is popular for its aroma and biological properties like as anti-nociceptive, antimicrobial, anticonvulsant and mosquito repellent[9-13]. In the present study the chemical composition of essential oil isolated from the roots of Cymbopogon winterianus Jowitt was investigated by GC/MS method which has not been exploited before.

EXPERIMENTAL

Collection of Plant Material

Fresh roots of Cymbopogon winterianus Jowitt were collected from Dr. Shushila Tiwari herbal garden Rishikesh, India in April, 2012. The plant was taxonomically identified and authenticated by the Botanical Survey of India, Dehradun, Uttarakhand by receiving a voucher specimen (Acc. No. 114828).

Isolation Procedure

Fresh roots of plant were washed in tap water and shade dried for 30 days. Dry roots were crushed by using a mechanical blender. 50gm of crushed roots of Cymbopogon winterianus Jowitt were subjected to steam distillation for 8 h by using a Clevenger apparatus (Clevenger, 1928). The oil was extracted from the distillate with n-hexane and dried over anhydrous sodium sulfate. The isolated oil was stored in an airtight dark colored bottle with proper labeling for GC/MS analysis.

Gas Chromatography-Mass Spectrometry Analysis

The essential oil from the roots of Cymbopogon winterianus Jowitt was analyzed on a Shimadzu QP-2010 (Shimadzu Corporation, Japan) system comprising an autosampler and gas chromatograph coupled to a mass spectrometer (GC/MS) employing the following conditions: Rxi-5 Sil MS cross bond, selectively composed of 5% diphenyl/ 95% dimethyl polysiloxate capillary column (30 m length x 0.25mm diameter x 0.10 µm thickness), helium (99.999% purity) was used as carrier gas at a constant flow of 0.7 ml/min and an injection volume of 1.0 µl of diluted oil in n-hexane was employed (split injection ratio of 1:20), injector temperature 250°C and ion source temperature 200°C. The GC oven temperature was programmed from 50°C (5 min) to 280°C (10 min) at a rate of 4°C/min. The mass spectra were taken at 70 eV (EI mode) with scanning range of m/z 30-600 (interface line temperature 300°C).

Identification of Compounds

The individual constituents of essential oil were identified by computerized matching of their mass spectra and retention indices with those gathered in the NIST 08, FFNS 1.2 and WILEY 8-Mass Spectral libraries of the GC/MS data system.

RESULTS AND DISCUSSION

The volatile oil content obtained from the roots of Java citronella was 0.16% v/w, and it exhibited yellow color with lemony odor. The results of chemical composition study of essential oil from the roots of Cymbopogon winterianus Jowitt are shown in Table 1. The major constituents were α-elemol (32.26%), guaiol (18.81%), methylcyclohexane (9.24%), γ-eudesmol (8.53%), τ-muurolol (6.83%), β-elemene (6.37%), δ-cadinene (4.23%) and (+)-citronellol (2.56%).

Table 1. Chemical composition of essential oil obtained from the roots of Cymbopogon winterianus Jowitt

No.	Compound	RT[a]	% Area	MW[b]	MF[c]
1.	Methyl cyclohexane	2.667	9.24	98	C_7H_{14}
2.	Ethyl cyclohexane	2.717	0.77	98	C_7H_{14}
3.	1,2,4-Trimethyl cyclohexane	2.763	0.44	112	C_8H_{16}
4.	Benzene, methyl-	2.983	0.94	92	C_7H_8
5.	1,3-Dimethylcyclohexane	3.137	0.92	112	C_8H_{16}
6.	Nonane	3.360	0.75	128	C_9H_{20}
7.	(+)-Citronellol	16.697	2.56	156	$C_{10}H_{20}O$
8.	β-Elemene	21.360	6.37	204	$C_{15}H_{24}$
9.	E-Germacrene D	23.693	1.34	204	$C_{15}H_{24}$
10.	β-Selinene	23.890	0.85	204	$C_{15}H_{24}$
11.	α-Muurolene	24.197	1.37	204	$C_{15}H_{24}$
12.	γ-Cadinene	24.557	1.84	204	$C_{15}H_{24}$
13.	δ-Cadinene	24.763	4.23	204	$C_{15}H_{24}$
14.	α-Elemol	25.713	32.26	222	$C_{15}H_{26}O$
15.	cis-Nerolidol	27.130	1.59	222	$C_{15}H_{26}O$
16.	γ-Eudesmol	27.670	8.53	222	$C_{15}H_{26}O$
17.	τ- Muurolol	27.810	6.83	222	$C_{15}H_{26}O$
18.	Guaiol	28.297	18.81	222	$C_{15}H_{26}O$
Total Identified Constituents		**100.00 %**			

[a] Retention Index relative to C_5-C_{32} n-alkanes as standaed; Rxi-5 Sil MS column; identification was done by GC/MS library

[b] Molecular mass

[c] Molecular formula

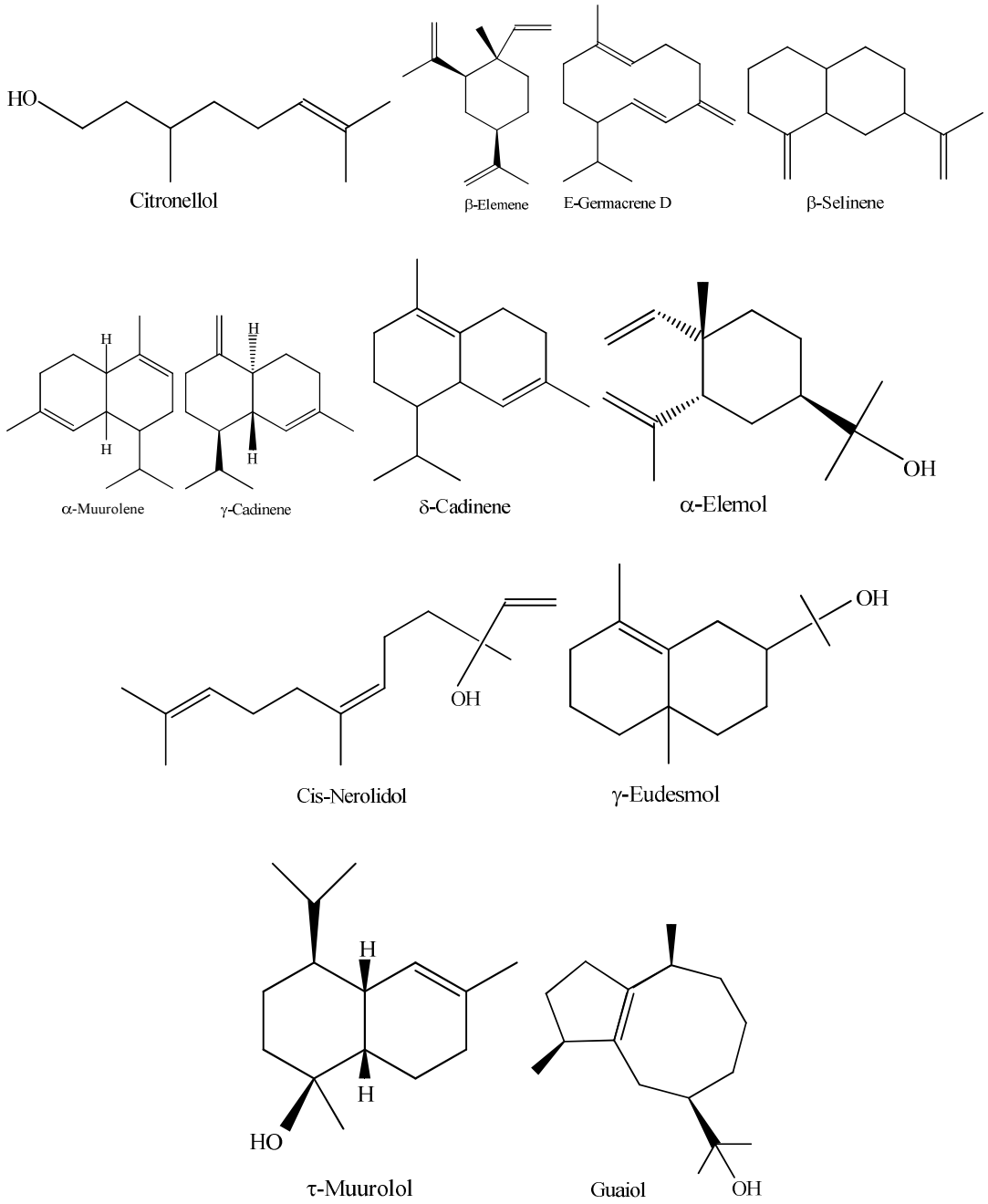

Figure 1. Structures of identified sesquiterpenes from the essential oil of Cymbopogon winterianus Jowitt roots

α-Elemol was found as a major constituent, reported as a floral odorous chemical and make the oil applications in soap and perfumery as fixatives (H. R. Ansari *at el*., 1974). Guaiol is used in the synthesis of some important chemicals like as guaiazulene which is an anti-inflammatory[15]. γ-Eudesmol has been reported as a perfumery chemical with sweet-woody and warm odor[14,16]. τ-Muurolol has been reported for its antioxidant, anti-cancer and antifungal properties[17-19]. β-Elemene is a floral compound with sweet odor and reported as a potential chemopreventive anti-cancer agent[20-21]. δ-Cadinene is a natural enzyme which participates in terpenoid biosynthesis[22]. (+)-Citronellol has been reported as a fragrance and mosquito repellents chemical[23]. Nerolidol is an important flavoring and perfumery chemical with a woody floral aroma. It also used as a skin penetration enhancer for the transdermal delivery of drugs[24-25]. E-Germacrene D has a faint, sweet-woody odor which is an important insect pheromone[14].

Results showed the most identified compounds in the Cymbopogon winterianus Jowitt roots oil were sesquiterpenes hydrocarbons and accounted to 86.58% of the oil. The structures of identified sesquiterpenes are presented in Figure 1. The identified sesquiterpenes are the main aroma compounds and most of them are biologically active, therefore the oil may be a vital ingredient of soap, candles, cosmetics, perfumes and pharmaceuticals[14].

CONCLUSION

The essential oil from the roots of Cymbopogon winterianus Jowitt was isolated by steam-distillation and analyzed by gas chromatography-mass spectrometry (GC/MS). Results showed that twelve sesquiterpenes which accounts to 86.58% of the oil were isolated from the essential oil of java citronella roots. Sesquiterpenes may be accountable for the biological properties of the oil. The results conclude the identified sesquiterpenes in essential oil studied possess characteristic aroma and several biological active compounds; hence the oil may be used widely in soaps, candles, flavors, fragrances, pharmaceuticals and in aromatherapy.

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